



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:23 AM GMT

PDB ID : 3MO2
Title : human G9a-like (GLP, also known as EHMT1) in complex with inhibitor E67
Authors : Chang, Y.; Horton, J.R.; Cheng, X.
Deposited on : 2010-04-22
Resolution : 2.49 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

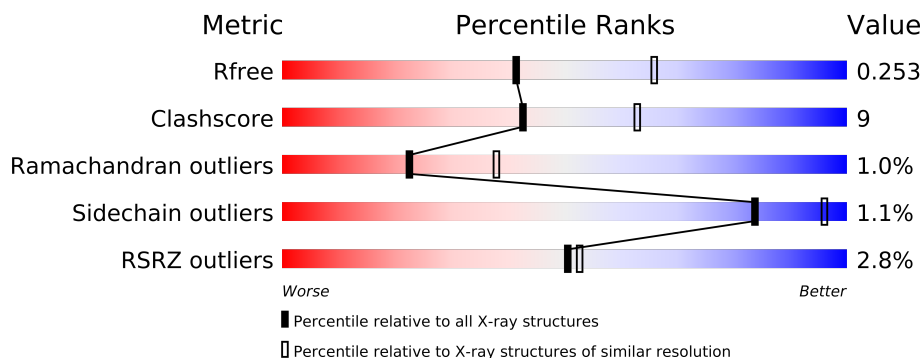
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	
1	D	285	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8719 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

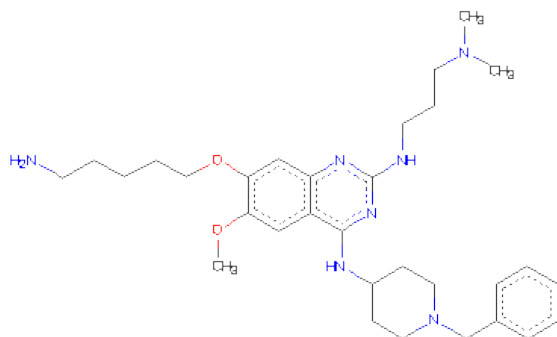
- Molecule 1 is a protein called Histone-lysine N-methyltransferase, H3 lysine-9 specific 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2016	1259	363	370	24			
1	B	258	Total	C	N	O	S	0	0	0
			2046	1279	367	375	25			
1	C	258	Total	C	N	O	S	0	0	0
			2040	1274	365	376	25			
1	D	256	Total	C	N	O	S	0	0	0
			1992	1249	353	365	25			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

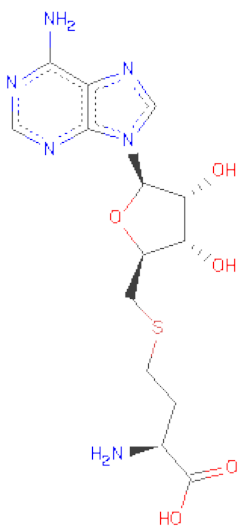
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Zn	0	0
			4	4		
2	A	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		

- Molecule 3 is 7-[(5-AMINOPENTYL)OXY]-N 4 -(1-BENZYLPIPERIDIN-4-YL)-N 2 -[3-(DIMETHYLAMINO)PROPYL]-6-METHOXYQUINAZOLINE-2,4-DIAMINE (three-letter code: E67) (formula: C₃₁H₄₇N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			40	31	7	2		
3	B	1	Total	C	N	O	0	0
			40	31	7	2		
3	C	1	Total	C	N	O	0	0
			40	31	7	2		
3	D	1	Total	C	N	O	0	0
			40	31	7	2		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 5 is water.

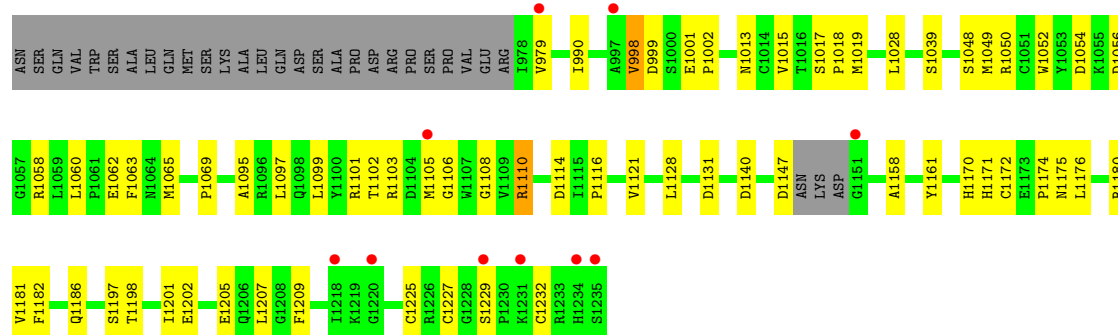
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	107	Total	O	0	0
			107	107		
5	C	114	Total	O	0	0
			114	114		
5	D	66	Total	O	0	0
			66	66		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

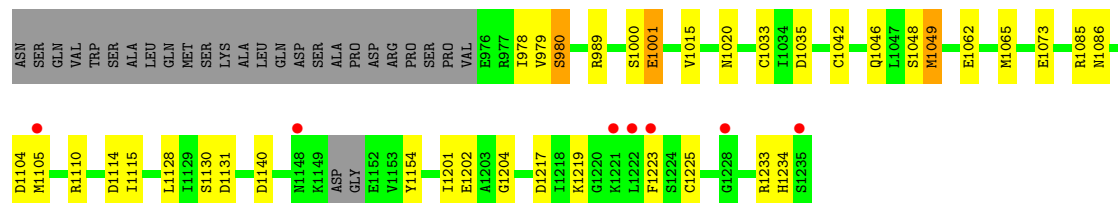
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain A: 



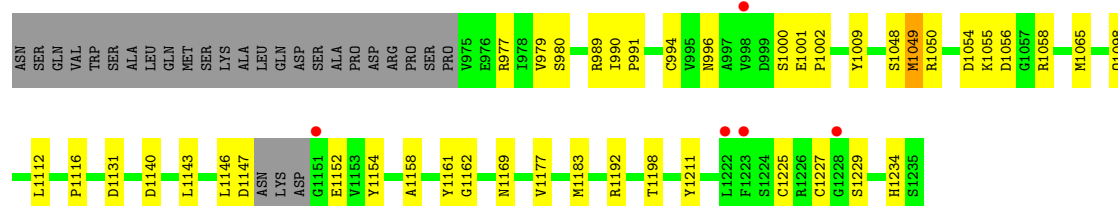
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain B: 




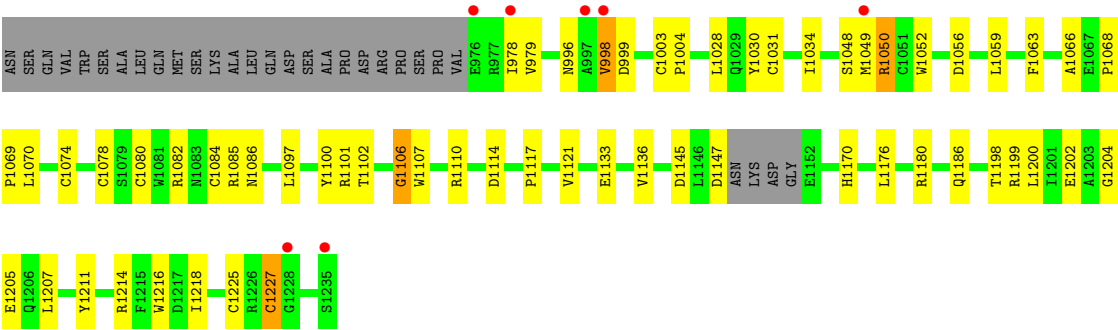
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain C: 



- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.70Å 163.00Å 69.30Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	31.83 – 2.49 31.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.5 (31.83-2.49) 91.4 (31.82-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.192 , 0.248 0.204 , 0.253	Depositor DCC
R_{free} test set	2107 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 43214 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAH, E67

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/2066	0.58	0/2800
1	B	0.36	0/2096	0.58	0/2839
1	C	0.36	0/2090	0.58	0/2832
1	D	0.34	0/2042	0.56	0/2774
All	All	0.35	0/8294	0.57	0/11245

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2016	0	1871	50	0
1	B	2046	0	1906	25	0
1	C	2040	0	1892	29	0
1	D	1992	0	1824	39	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	40	0	47	3	0
3	B	40	0	47	2	0
3	C	40	0	47	3	0
3	D	40	0	47	0	0
4	C	26	0	19	0	0
4	D	26	0	20	0	0
5	A	110	0	0	2	0
5	B	107	0	0	0	0
5	C	114	0	0	1	0
5	D	66	0	0	2	0
All	All	8719	0	7720	142	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (142) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1001:GLU:HB3	1:A:1101:ARG:HH12	1.42	0.83
1:C:980:SER:HB3	1:C:994:CYS:HB3	1.66	0.77
1:B:1062:GLU:OE1	1:B:1062:GLU:N	2.20	0.74
1:D:1170:HIS:CD2	1:D:1216:TRP:HE1	2.06	0.73
1:D:1031:CYS:SG	5:D:295:HOH:O	2.46	0.72
1:B:978:ILE:H	1:B:978:ILE:HD12	1.53	0.71
1:A:1001:GLU:HB3	1:A:1101:ARG:NH1	2.05	0.70
1:D:1114:ASP:OD1	1:D:1202:GLU:HA	1.93	0.68
1:C:1131:ASP:OD1	3:C:1236:E67:HAWA	1.93	0.67
1:A:1140:ASP:O	3:A:1:E67:HAMA	1.94	0.67
1:D:1170:HIS:CD2	1:D:1211:TYR:H	2.13	0.66
1:B:1048:SER:O	1:B:1049:MET:HB2	1.94	0.66
1:A:998:VAL:HG21	1:A:1102:THR:O	1.97	0.65
1:B:989:ARG:HG2	1:B:989:ARG:HH11	1.62	0.65
1:A:1001:GLU:CB	1:A:1101:ARG:HH12	2.09	0.65
1:A:1048:SER:O	1:A:1049:MET:HB2	1.97	0.64
1:C:1065:MET:HE3	1:C:1198:THR:HA	1.79	0.64
1:A:1114:ASP:OD1	1:A:1202:GLU:HA	1.98	0.64
1:D:1133:GLU:O	1:D:1136:VAL:HG12	1.99	0.62
1:A:1052:TRP:O	1:A:1060:LEU:HD13	2.00	0.61
1:B:1131:ASP:OD2	3:B:2:E67:HAWA	2.01	0.61
1:D:1100:TYR:CE1	1:D:1102:THR:HG22	2.36	0.60
1:D:1225:CYS:SG	1:D:1227:CYS:HB3	2.43	0.59
1:D:1048:SER:O	1:D:1049:MET:HB2	2.03	0.58
1:C:1065:MET:CE	1:C:1198:THR:HA	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1117:PRO:HG3	1:D:1200:LEU:N	2.20	0.57
1:B:1015:VAL:HG12	1:B:1128:LEU:HB3	1.86	0.57
1:A:1121:VAL:HG21	1:A:1176:LEU:HD21	1.88	0.56
1:A:1225:CYS:SG	1:A:1227:CYS:HB3	2.45	0.56
1:D:1170:HIS:HD2	1:D:1211:TYR:H	1.54	0.55
1:B:1219:LYS:HB3	1:B:1223:PHE:CZ	2.42	0.55
1:D:998:VAL:HG12	1:D:999:ASP:N	2.22	0.54
1:D:1145:ASP:OD2	1:D:1214:ARG:HD2	2.08	0.54
1:A:1101:ARG:HD2	1:A:1106:GLY:O	2.08	0.54
1:A:1054:ASP:OD1	1:A:1056:ASP:N	2.41	0.54
1:A:1028:LEU:HD23	1:A:1186:GLN:HG3	1.90	0.54
1:D:1034:ILE:HD12	1:D:1034:ILE:C	2.29	0.53
1:C:979:VAL:HG21	1:C:1002:PRO:HA	1.90	0.53
1:B:978:ILE:N	1:B:978:ILE:HD12	2.21	0.53
1:B:1114:ASP:OD1	1:B:1202:GLU:HA	2.09	0.53
1:B:1085:ARG:HA	1:C:1055:LYS:HD2	1.92	0.52
1:C:1048:SER:O	1:C:1049:MET:HB2	2.09	0.52
1:D:1110:ARG:HD2	1:D:1204:GLY:HA2	1.91	0.52
1:B:989:ARG:HG2	1:B:989:ARG:NH1	2.24	0.52
1:A:1065:MET:CE	1:A:1198:THR:HA	2.40	0.52
1:A:1097:LEU:HD22	1:A:1207:LEU:HD11	1.92	0.51
1:C:979:VAL:O	1:C:979:VAL:HG22	2.11	0.51
1:A:998:VAL:HG12	1:A:999:ASP:N	2.24	0.50
1:D:996:ASN:ND2	1:D:999:ASP:O	2.45	0.50
1:B:1110:ARG:HD3	1:B:1204:GLY:HA2	1.92	0.50
1:D:1101:ARG:NH1	1:D:1106:GLY:HA2	2.27	0.50
1:D:1202:GLU:O	1:D:1205:GLU:HB2	2.11	0.49
1:B:1225:CYS:HB2	1:B:1234:HIS:HB2	1.94	0.49
1:A:1174:PRO:HB3	1:A:1209:PHE:HA	1.93	0.49
1:A:1101:ARG:HE	1:A:1105:MET:C	2.14	0.49
1:A:1172:CYS:SG	1:A:1232:CYS:HA	2.53	0.49
1:C:979:VAL:HG12	1:C:994:CYS:O	2.12	0.48
1:B:978:ILE:H	1:B:978:ILE:CD1	2.25	0.48
1:C:1065:MET:SD	1:C:1177:VAL:HG11	2.54	0.48
1:A:979:VAL:O	1:A:979:VAL:HG12	2.12	0.48
1:A:1181:VAL:HG12	1:A:1182:PHE:N	2.29	0.48
1:A:1028:LEU:CD2	1:A:1186:GLN:HG3	2.44	0.48
1:A:1015:VAL:HG12	1:A:1128:LEU:HB3	1.96	0.48
1:B:1115:ILE:HB	1:B:1201:ILE:HB	1.97	0.47
1:C:1000:SER:O	1:C:1001:GLU:C	2.52	0.47
1:A:1060:LEU:HB3	1:A:1062:GLU:OE1	2.13	0.47
1:A:979:VAL:HG11	1:A:1002:PRO:HA	1.94	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1175:ASN:O	1:A:1197:SER:HA	2.14	0.47
1:C:1098:GLN:NE2	1:C:1112:LEU:HD21	2.28	0.47
1:C:1140:ASP:HB3	3:C:1236:E67:HATA	1.96	0.47
1:C:990:ILE:HG23	1:C:991:PRO:HD2	1.95	0.47
1:A:1174:PRO:CB	1:A:1209:PHE:HA	2.45	0.47
1:B:1073:GLU:HA	1:B:1086:ASN:ND2	2.29	0.47
1:D:1121:VAL:HG21	1:D:1176:LEU:HD21	1.96	0.47
1:C:1169:ASN:HA	1:C:1211:TYR:OH	2.15	0.47
1:A:1158:ALA:HA	1:A:1161:TYR:O	2.15	0.46
1:A:990:ILE:HD11	1:A:1095:ALA:O	2.15	0.46
1:D:1063:PHE:CZ	1:D:1069:PRO:HD2	2.51	0.46
1:D:1048:SER:C	1:D:1050:ARG:H	2.18	0.46
1:C:989:ARG:HH11	1:C:989:ARG:HG2	1.81	0.46
1:B:1000:SER:O	1:B:1001:GLU:C	2.54	0.46
1:A:1131:ASP:OD1	3:A:1:E67:HAWA	2.15	0.46
1:A:1058:ARG:NE	1:A:1116:PRO:HB2	2.31	0.46
1:A:1017:SER:HB2	1:A:1018:PRO:CD	2.46	0.45
1:A:1110:ARG:HB2	1:A:1205:GLU:O	2.16	0.45
1:A:1013:ASN:HB2	5:A:228:HOH:O	2.15	0.45
1:D:1004:PRO:HD3	1:D:1107:TRP:CZ2	2.52	0.45
1:A:999:ASP:OD1	1:A:1101:ARG:NH1	2.50	0.45
1:D:1214:ARG:O	1:D:1218:ILE:HG13	2.17	0.45
1:D:1066:ALA:O	1:D:1068:PRO:HD3	2.16	0.45
1:B:1033:CYS:HB3	1:B:1035:ASP:OD1	2.17	0.44
1:C:1050:ARG:NH1	5:C:292:HOH:O	2.49	0.44
1:C:977:ARG:HG2	1:C:996:ASN:O	2.17	0.44
1:D:1117:PRO:HG3	1:D:1199:ARG:C	2.37	0.44
1:D:1097:LEU:HD22	1:D:1207:LEU:HD11	1.99	0.44
1:B:979:VAL:O	1:B:980:SER:HB2	2.17	0.44
1:C:1058:ARG:HE	1:C:1116:PRO:HB2	1.83	0.44
1:D:1176:LEU:HD11	1:D:1207:LEU:HB3	2.00	0.44
1:D:1028:LEU:HD23	1:D:1186:GLN:HG3	2.00	0.44
1:C:1183:MET:HE3	1:C:1192:ARG:HD3	1.99	0.43
1:A:1114:ASP:HA	1:A:1201:ILE:O	2.18	0.43
1:A:1065:MET:HE1	1:A:1198:THR:HA	2.01	0.43
1:C:1048:SER:O	1:C:1049:MET:CB	2.66	0.43
1:C:1227:CYS:SG	1:C:1229:SER:HB3	2.58	0.43
1:A:1019:MET:HA	5:A:269:HOH:O	2.18	0.43
1:D:1117:PRO:HG3	1:D:1199:ARG:HA	2.01	0.43
1:A:1099:LEU:HD12	1:A:1108:GLY:O	2.18	0.43
1:A:1103:ARG:C	1:A:1105:MET:H	2.21	0.43
1:C:1158:ALA:HA	1:C:1161:TYR:O	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1180:ARG:HG3	1:A:1180:ARG:HH11	1.84	0.43
1:B:1062:GLU:H	1:B:1062:GLU:CD	2.17	0.42
1:D:1170:HIS:HD2	1:D:1211:TYR:HB2	1.84	0.42
1:D:1110:ARG:HB2	1:D:1205:GLU:O	2.19	0.42
1:A:1065:MET:HE3	1:A:1198:THR:HA	2.01	0.42
1:D:1080:CYS:HA	5:D:263:HOH:O	2.18	0.42
1:A:1227:CYS:SG	1:A:1229:SER:HB3	2.59	0.42
1:B:1233:ARG:NH1	1:B:1233:ARG:HB2	2.34	0.42
1:B:1104:ASP:O	1:B:1105:MET:HB2	2.19	0.42
1:A:1058:ARG:HH21	1:A:1116:PRO:HD2	1.83	0.42
1:A:1048:SER:C	1:A:1050:ARG:H	2.23	0.42
1:C:1146:LEU:O	1:C:1147:ASP:C	2.56	0.42
1:A:1058:ARG:HE	1:A:1116:PRO:HB2	1.84	0.42
1:D:1070:LEU:HD21	1:D:1180:ARG:CZ	2.50	0.41
1:D:979:VAL:CB	1:D:1003:CYS:HB2	2.50	0.41
1:B:1042:CYS:O	1:B:1046:GLN:HG3	2.21	0.41
1:C:1054:ASP:OD1	1:C:1056:ASP:N	2.54	0.41
1:B:1140:ASP:OD2	3:B:2:E67:HAC	2.21	0.41
1:A:1170:HIS:CG	1:A:1171:HIS:N	2.88	0.41
1:D:1052:TRP:O	1:D:1059:LEU:HA	2.20	0.41
1:A:1054:ASP:OD1	1:A:1054:ASP:C	2.60	0.41
1:C:1143:LEU:O	3:C:1236:E67:HBE	2.21	0.40
1:D:1074:CYS:SG	1:D:1086:ASN:HB3	2.61	0.40
1:C:1225:CYS:HB2	1:C:1234:HIS:HB2	2.03	0.40
1:B:1130:SER:HA	1:B:1154:TYR:CD1	2.56	0.40
1:D:1170:HIS:HB2	1:D:1211:TYR:CD1	2.56	0.40
1:A:1140:ASP:OD2	3:A:1:E67:HAC	2.21	0.40
1:D:1198:THR:O	1:D:1199:ARG:HB3	2.21	0.40
1:C:1009:TYR:HA	1:C:1162:GLY:O	2.21	0.40
1:A:1063:PHE:CZ	1:A:1069:PRO:HD2	2.56	0.40
1:D:1030:TYR:HB2	1:D:1078:CYS:HA	2.04	0.40
1:D:1082:ARG:HG3	1:D:1082:ARG:O	2.22	0.40
1:C:1152:GLU:HG2	1:C:1154:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/285 (88%)	226 (90%)	24 (10%)	1 (0%)	43	66
1	B	254/285 (89%)	233 (92%)	17 (7%)	4 (2%)	14	23
1	C	254/285 (89%)	229 (90%)	24 (9%)	1 (0%)	43	66
1	D	252/285 (88%)	221 (88%)	27 (11%)	4 (2%)	14	23
All	All	1011/1140 (89%)	909 (90%)	92 (9%)	10 (1%)	22	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	998	VAL
1	B	980	SER
1	B	1020	ASN
1	C	1049	MET
1	D	1106	GLY
1	D	1050	ARG
1	B	1001	GLU
1	B	1049	MET
1	D	978	ILE
1	A	998	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	219/257 (85%)	216 (99%)	3 (1%)	78	94
1	B	223/257 (87%)	221 (99%)	2 (1%)	87	97
1	C	222/257 (86%)	222 (100%)	0	100	100
1	D	213/257 (83%)	208 (98%)	5 (2%)	63	87
All	All	877/1028 (85%)	867 (99%)	10 (1%)	84	96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1039	SER
1	A	1110	ARG
1	A	1147	ASP
1	B	1065	MET
1	B	1217	ASP
1	D	1056	ASP
1	D	1084	CYS
1	D	1085	ARG
1	D	1147	ASP
1	D	1227	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1064	ASN
1	A	1234	HIS
1	D	1041	ASN
1	D	1170	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	E67	A	1	-	43,43,43	1.87	11 (25%)	56,56,56	1.98	13 (23%)
3	E67	B	2	-	43,43,43	1.89	11 (25%)	56,56,56	1.96	11 (19%)
4	SAH	C	103	-	28,28,28	1.06	4 (14%)	40,40,40	3.66	8 (20%)
3	E67	C	1236	-	43,43,43	1.91	10 (23%)	56,56,56	1.95	11 (19%)
4	SAH	D	104	-	28,28,28	1.34	3 (10%)	40,40,40	2.96	8 (20%)
3	E67	D	4	-	43,43,43	1.87	11 (25%)	56,56,56	1.82	11 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E67	A	1	-	-	0/24/34/34	0/2/4/4
3	E67	B	2	-	-	0/24/34/34	0/2/4/4
4	SAH	C	103	-	-	0/15/31/31	0/1/3/3
3	E67	C	1236	-	-	0/24/34/34	0/2/4/4
4	SAH	D	104	-	-	0/15/31/31	0/1/3/3
3	E67	D	4	-	-	0/24/34/34	0/2/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	E67	CBL-CBM	5.32	1.53	1.37
3	D	4	E67	CBL-CBM	5.27	1.53	1.37
3	C	1236	E67	CBL-CBM	5.21	1.53	1.37
3	A	1	E67	CBL-CBM	5.16	1.52	1.37
3	C	1236	E67	CBK-CBL	4.56	1.51	1.37
4	D	104	SAH	OXT-C	4.56	1.46	1.30
3	A	1	E67	CBK-CBL	4.48	1.50	1.37
3	B	2	E67	CBK-CBL	4.48	1.50	1.37
3	D	4	E67	CAC-CAB	4.33	1.44	1.36
3	D	4	E67	CBK-CBL	4.31	1.50	1.37
3	B	2	E67	CAF-CAA	4.17	1.44	1.36
3	D	4	E67	CAF-CAA	3.96	1.43	1.36
3	A	1	E67	CAF-CAA	3.94	1.43	1.36
3	C	1236	E67	CAF-CAA	3.91	1.43	1.36
3	C	1236	E67	CAC-CAB	3.90	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	E67	CAC-CAB	3.83	1.43	1.36
3	A	1	E67	CAC-CAB	3.73	1.43	1.36
4	D	104	SAH	C4-N9	-3.25	1.33	1.37
4	C	103	SAH	C4-N9	-3.11	1.33	1.37
3	A	1	E67	C6-C5	-2.95	1.41	1.45
3	B	2	E67	C6-C5	-2.91	1.41	1.45
3	A	1	E67	CBH-CBI	2.90	1.56	1.51
3	C	1236	E67	C6-C5	-2.85	1.41	1.45
3	C	1236	E67	CBH-CBI	2.78	1.56	1.51
3	B	2	E67	CBJ-CBI	2.74	1.45	1.38
3	C	1236	E67	CBJ-CBI	2.70	1.45	1.38
3	D	4	E67	CBH-CBI	2.68	1.56	1.51
3	A	1	E67	CBJ-CBI	2.64	1.44	1.38
3	C	1236	E67	CAP-CAQ	2.64	1.60	1.52
3	B	2	E67	CBH-CBI	2.58	1.56	1.51
3	B	2	E67	CAP-CAQ	2.52	1.59	1.52
3	D	4	E67	CBJ-CBI	2.51	1.44	1.38
3	D	4	E67	C6-C5	-2.46	1.41	1.45
3	C	1236	E67	CBN-CBI	2.45	1.44	1.38
3	A	1	E67	CBN-CBI	2.34	1.44	1.38
3	A	1	E67	CAP-CAQ	2.33	1.59	1.52
4	C	103	SAH	O4'-C1'	2.31	1.44	1.41
3	D	4	E67	CAP-CAQ	2.30	1.59	1.52
3	D	4	E67	C6-N1	2.29	1.36	1.33
3	B	2	E67	CBN-CBI	2.24	1.43	1.38
3	D	4	E67	CBN-CBI	2.23	1.43	1.38
4	D	104	SAH	C8-N9	-2.23	1.33	1.36
4	C	103	SAH	C8-N9	-2.20	1.33	1.36
3	C	1236	E67	OAL-CAB	2.19	1.40	1.37
3	A	1	E67	C6-N1	2.18	1.36	1.33
3	D	4	E67	OAL-CAB	2.18	1.40	1.37
3	A	1	E67	CBH-NAR	2.18	1.51	1.47
3	B	2	E67	OAL-CAB	2.12	1.40	1.37
4	C	103	SAH	C5-N7	-2.03	1.32	1.40
3	B	2	E67	CAW-CAX	-2.02	1.43	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	103	SAH	OXT-C-CA	14.39	149.16	116.88
4	C	103	SAH	OXT-C-O	-13.60	93.32	124.07
4	D	104	SAH	OXT-C-O	-10.81	99.62	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	104	SAH	OXT-C-CA	9.52	138.23	116.88
4	C	103	SAH	N3-C2-N1	-8.50	121.61	128.71
4	D	104	SAH	N3-C2-N1	-8.41	121.68	128.71
3	B	2	E67	CAC-C5-C6	-7.26	121.08	124.98
3	A	1	E67	CAC-C5-C6	-7.22	121.11	124.98
3	C	1236	E67	CAC-C5-C6	-7.17	121.13	124.98
3	D	4	E67	CAC-C5-C6	-6.43	121.53	124.98
3	B	2	E67	CAV-NAU-C2	-5.92	112.63	123.67
3	C	1236	E67	CAV-NAU-C2	-5.70	113.03	123.67
3	A	1	E67	C6-C5-C4	5.50	118.76	115.63
3	A	1	E67	CAV-NAU-C2	-5.47	113.47	123.67
3	B	2	E67	C6-C5-C4	5.38	118.69	115.63
3	C	1236	E67	C6-C5-C4	5.14	118.56	115.63
3	D	4	E67	CAV-NAU-C2	-4.96	114.43	123.67
3	D	4	E67	C6-C5-C4	4.92	118.43	115.63
4	C	103	SAH	N3-C4-N9	4.53	133.61	125.43
4	D	104	SAH	N3-C4-N9	4.38	133.34	125.43
3	B	2	E67	CAW-CAX-NAY	-4.03	103.04	113.59
3	C	1236	E67	CAW-CAX-NAY	-3.93	103.31	113.59
3	A	1	E67	N3-C2-N1	-3.50	120.78	126.19
3	A	1	E67	CAW-CAX-NAY	-3.45	104.57	113.59
3	D	4	E67	CAW-CAX-NAY	-3.42	104.64	113.59
3	D	4	E67	N3-C2-N1	-3.40	120.94	126.19
3	C	1236	E67	N3-C2-N1	-3.27	121.14	126.19
3	B	2	E67	N3-C2-N1	-3.23	121.21	126.19
3	A	1	E67	C6-NAN-CAO	3.22	127.85	123.84
3	C	1236	E67	NAU-C2-N3	3.18	123.16	117.17
3	B	2	E67	C2-N1-C6	3.12	123.46	116.97
3	B	2	E67	NAU-C2-N3	3.11	123.04	117.17
3	C	1236	E67	C2-N1-C6	3.08	123.38	116.97
4	D	104	SAH	C5'-C4'-C3'	-3.07	107.03	114.98
4	C	103	SAH	C5'-C4'-C3'	-3.03	107.12	114.98
4	D	104	SAH	C5-C4-N3	-2.95	119.29	125.70
4	C	103	SAH	C5-C4-N3	-2.93	119.32	125.70
3	D	4	E67	C2-N1-C6	2.89	122.98	116.97
3	C	1236	E67	C5-C4-N3	-2.88	120.20	122.86
3	A	1	E67	NAU-C2-N3	2.80	122.46	117.17
3	A	1	E67	C2-N1-C6	2.76	122.70	116.97
3	B	2	E67	C5-C4-N3	-2.74	120.33	122.86
3	D	4	E67	NAU-C2-N3	2.68	122.22	117.17
3	A	1	E67	CBH-NAR-CAQ	-2.60	106.56	111.07
4	D	104	SAH	C4-C5-N7	-2.57	107.32	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	E67	CBH-NAR-CAQ	-2.53	106.68	111.07
3	A	1	E67	C5-C4-N3	-2.50	120.56	122.86
3	D	4	E67	C5-C4-N3	-2.49	120.57	122.86
4	C	103	SAH	C4-C5-N7	-2.36	107.50	109.52
3	A	1	E67	CBI-CBH-NAR	2.33	117.81	113.20
4	D	104	SAH	C2-N3-C4	2.31	120.60	114.01
3	C	1236	E67	OAL-CAB-CAC	-2.31	122.34	125.25
4	C	103	SAH	C2-N3-C4	2.30	120.56	114.01
3	B	2	E67	C5-C6-N1	-2.27	117.41	121.63
3	B	2	E67	OAL-CAB-CAC	-2.26	122.41	125.25
3	C	1236	E67	OAL-CAB-CAA	2.24	118.67	115.42
3	D	4	E67	CBI-CBH-NAR	2.20	117.55	113.20
3	D	4	E67	C5-C6-N1	-2.18	117.59	121.63
3	A	1	E67	OAL-CAB-CAC	-2.12	122.58	125.25
3	C	1236	E67	C5-C6-N1	-2.10	117.72	121.63
3	A	1	E67	C5-C6-N1	-2.09	117.74	121.63
3	B	2	E67	OAL-CAB-CAA	2.09	118.45	115.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	255/285 (89%)	0.03	10 (3%) 37 38	15, 35, 62, 71	0
1	B	258/285 (90%)	-0.13	7 (2%) 52 54	18, 33, 58, 70	0
1	C	258/285 (90%)	-0.11	5 (1%) 64 66	15, 33, 56, 66	0
1	D	256/285 (89%)	0.11	7 (2%) 52 54	23, 44, 64, 75	0
All	All	1027/1140 (90%)	-0.03	29 (2%) 50 53	15, 36, 61, 75	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1235	SER	5.1
1	B	1105	MET	4.6
1	D	998	VAL	3.8
1	D	976	GLU	3.6
1	A	1220	GLY	3.3
1	A	1151	GLY	3.1
1	A	1105	MET	3.0
1	C	998	VAL	3.0
1	C	1222	LEU	2.8
1	A	1218	ILE	2.6
1	A	1234	HIS	2.6
1	B	1235	SER	2.5
1	D	1235	SER	2.5
1	A	997	ALA	2.4
1	B	1148	ASN	2.3
1	A	979	VAL	2.3
1	D	1228	GLY	2.3
1	D	1049	MET	2.3
1	D	997	ALA	2.2
1	B	1222	LEU	2.2
1	C	1228	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1221	LYS	2.1
1	A	1229	SER	2.1
1	A	1231	LYS	2.1
1	B	1223	PHE	2.1
1	C	1223	PHE	2.1
1	B	1228	GLY	2.0
1	D	978	ILE	2.0
1	C	1151	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	E67	A	1	40/40	0.26	1.62	42,49,65,66	0
4	SAH	D	104	26/26	0.21	1.44	66,67,68,69	0
3	E67	C	1236	40/40	0.19	1.04	37,43,60,61	0
3	E67	D	4	40/40	0.22	0.83	40,49,63,64	0
3	E67	B	2	40/40	0.17	0.81	37,41,53,54	0
2	ZN	C	3	1/1	0.10	0.42	25,25,25,25	0
4	SAH	C	103	26/26	0.16	0.21	51,57,59,60	0
2	ZN	A	340	1/1	0.10	0.16	22,22,22,22	0
2	ZN	A	342	1/1	0.10	0.02	19,19,19,19	0
2	ZN	A	341	1/1	0.10	-0.23	18,18,18,18	0
2	ZN	B	6	1/1	0.10	-0.25	24,24,24,24	0
2	ZN	C	1	1/1	0.09	-0.31	26,26,26,26	0
2	ZN	C	2	1/1	0.08	-0.46	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	D	7	1/1	0.08	-0.93	37,37,37,37	0
2	ZN	D	6	1/1	0.09	-1.28	32,32,32,32	0
2	ZN	C	4	1/1	0.06	-1.33	46,46,46,46	0
2	ZN	B	5	1/1	0.08	-1.42	25,25,25,25	0
2	ZN	B	7	1/1	0.08	-1.50	31,31,31,31	0
2	ZN	B	8	1/1	0.06	-1.77	41,41,41,41	0
2	ZN	D	5	1/1	0.07	-1.80	37,37,37,37	0
2	ZN	A	343	1/1	0.06	-1.89	51,51,51,51	0
2	ZN	D	8	1/1	0.05	-2.10	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.